

Sundance: A High-Level Tool for PDE-Constrained Simulation and Optimization

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In this talk we describe Sundance, a software system for rapid development of parallel PDE simulation and optimization problems. Sundance was originally designed with PDE-constrained optimization in mind, but the features that make it suitable for use in PDE-constrained optimization turn out to also make it useful as a general-purpose research tool in PDE simulation.

Modern algorithms for PDE-constrained optimization require the application of operators and the solution of systems of equations that are different from those used in a single solution of the PDE, and require a closer degree of interaction between the PDE solver and optimizer than is usually available. Even with modern PDE frameworks such as Sandia's SIERRA and Nevada, it involves considerable development effort to obtain the quantities required for PDE-constrained optimization, and consequently the best algorithms for PDE-constrained optimization have been little used outside of academic research projects. Indeed, even research into these algorithms is hindered because of the considerable startup costs involved in writing a non-traditional PDE-simulator.

To facilitate research into, and application of, PDE-constrained optimization we have developed a general-purpose PDE solver system that has been designed from the ground up with large-scale, parallel, PDE-constrained optimization in mind. This system, called Sundance, accepts a system of coupled PDEs and boundary conditions written in symbolic form that is close to the notation in which a scientist or engineer would normally write them with pencil and paper. Each function or variation appearing in this symbolic description is annotated with a specification of the finite-element basis with which that object will be discretized. This information, along with a mesh, is then used by Sundance to assemble the implied discretized operators.

The symbolic interface to Sundance makes it quite simple to develop a high-performance code to create the non-traditional operators seen in PDE-constrained optimization. Furthermore, this symbolic interface is essentially a rapid-development tool that can be used for exploration of new solver algorithms, physical models, or finite-element formulations that are not available in standard codes.